Thiamine disulfide

67-16-3 | DTXSID6046890

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1360 L/kg

Global applicability domain: Outside

Local applicability domain index: 1.34e-01

Confidence level: 6.07e-01

Nearest Neighbors from the Training Set

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Triflusulfuron-methyl
Measured: 69.2
Predicted: 50.2

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Hydramethylnon
Measured: 724000
Predicted: 425000

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Fluvalinate
Measured: 507000
Predicted: 293000

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tau-Fluvalinate
Measured: 507000
Predicted: 284000

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Nicosulfuron
Measured: 30.2
Predicted: 53.4

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Primisulfuron-methyl
Measured: 12.0
Predicted: 48.2